Learning From Data
Lecture 8
Linear Classification and Regression

Linear Classification
Linear Regression

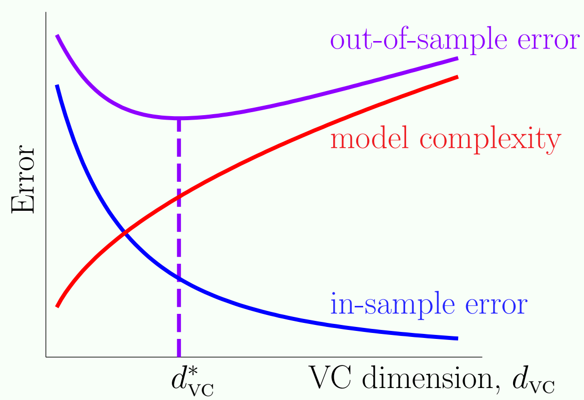
M. Magdon-Ismail
CSCI 4100/6100

RECAP: **Approximation Versus Generalization**

VC Analysis

$$E_{\text{out}} \leq E_{\text{in}} + \Omega(d_{\text{VC}})$$

1. Did you fit your data well enough (E_{in})?
2. Are you confident your E_{in} will generalize to E_{out}



The VC Insuarance Co.

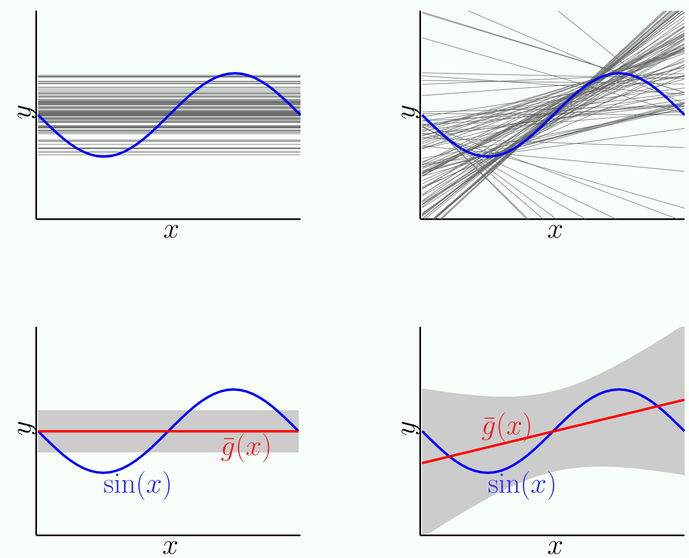
The VC bound is like a warranty.

If you look at your data *before* choosing $\mathcal{H}$, your warranty is void.

Bias-Variance Analysis

$$E_{\text{out}} = \text{bias} + \text{var}$$

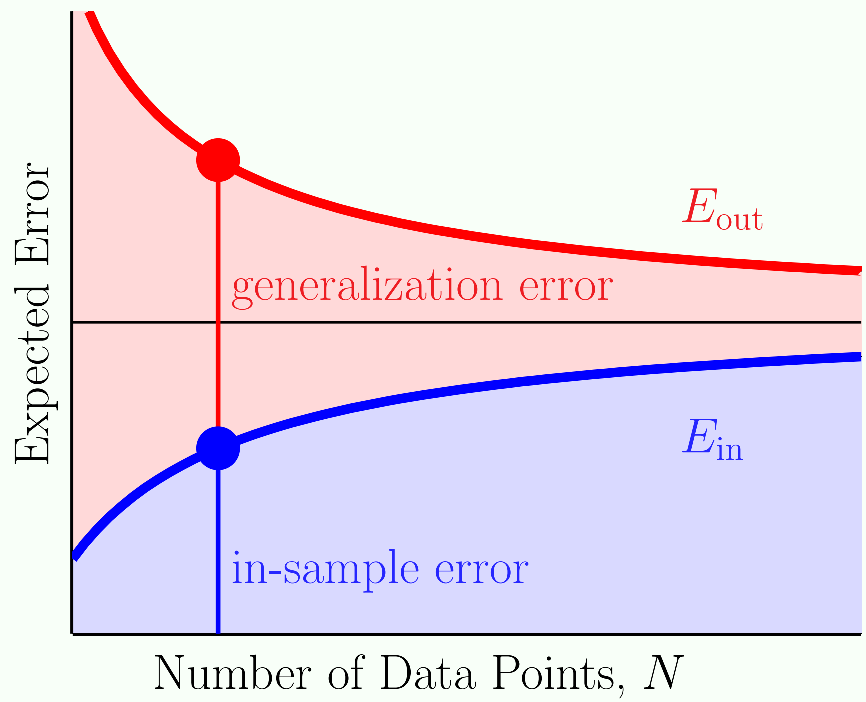
1. How well can you fit your data (bias)?
2. How close to that best fit can you get (var)?



$\mathcal{H}_0$	$\mathcal{H}_1$
bias $= 0.50$;	bias $= 0.21$;
var $= 0.25$.	var $= 1.69$.
$E_{\text{out}} = 0.75$ ✓	$E_{\text{out}} = 1.90$

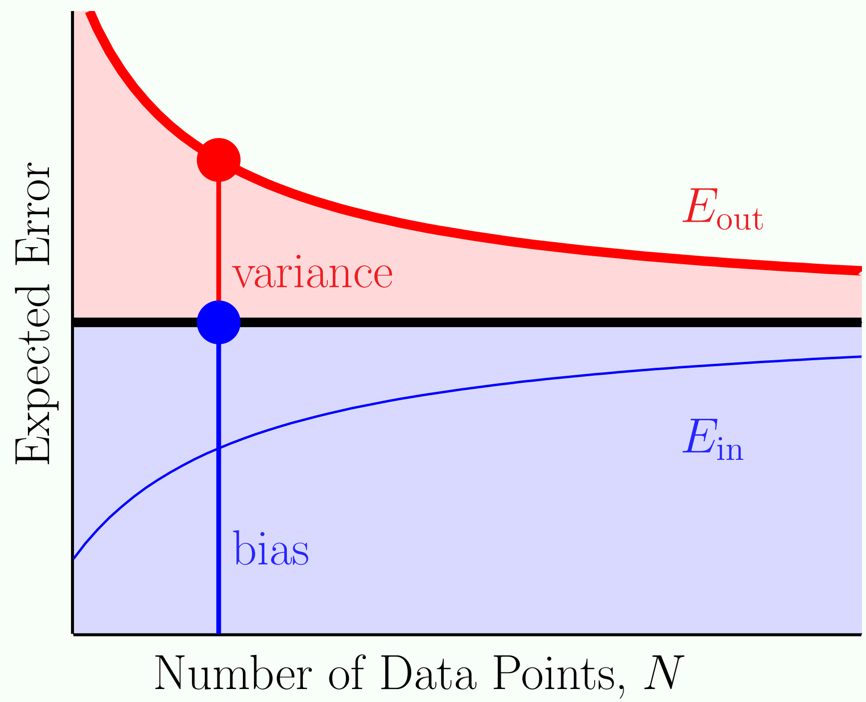
Decomposing The Learning Curve

VC Analysis



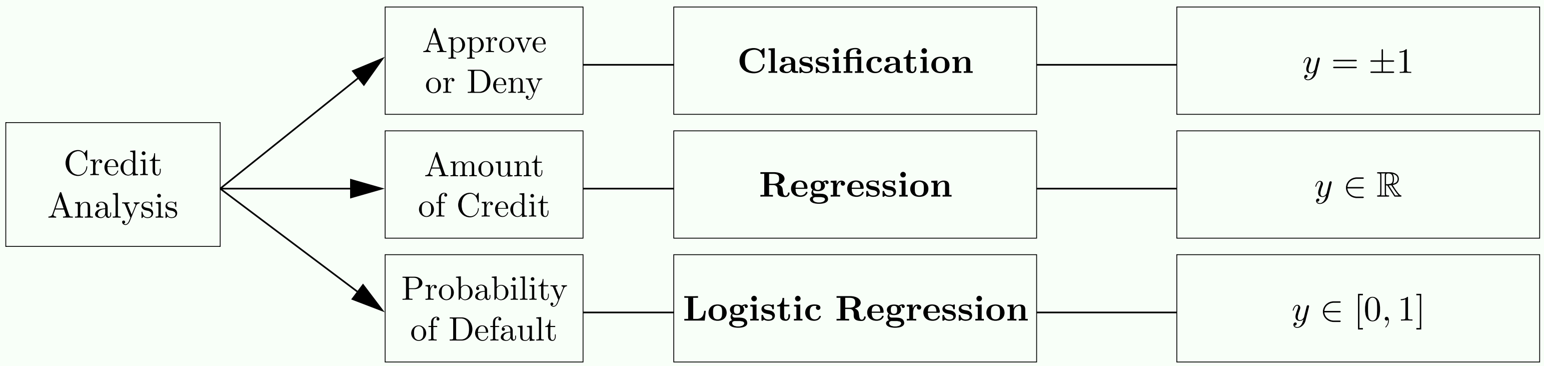
Pick $\mathcal{H}$ that can generalize and has a good chance to fit the data

Bias-Variance Analysis



Pick $(\mathcal{H}, \mathcal{A})$ to approximate f and not behave wildly after seeing the data

Three Learning Problems



- Linear models are perhaps ***the*** fundamental model.

- The linear model is the first model to try.

The Linear Signal

linear in $\mathbf{x}$: gives the line/hyperplane separator

$$\downarrow$$

$$s = \mathbf{w}^{\mathrm{T}}\mathbf{x}$$

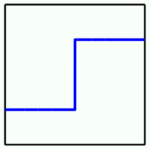
$$\uparrow$$

linear in $\mathbf{w}$: makes the algorithms work

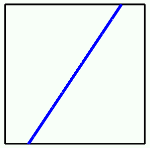
$\mathbf{x}$ is the augmented vector: $\mathbf{x} \in \{1\} \times \mathbb{R}^d$

The Linear Signal

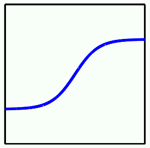
$$s = \mathbf{w}^{\mathrm{T}}\mathbf{x} \longrightarrow \left\{ \begin{array}{l} \\ \\ \\ \end{array} \right.$$



$\rightarrow \; \mathrm{sign}(\mathbf{w}^{\mathrm{T}}\mathbf{x}) \qquad \{-1, +1\}$



$\rightarrow \; \mathbf{w}^{\mathrm{T}}\mathbf{x} \qquad \mathbb{R}$



$\rightarrow \; \theta(\mathbf{w}^{\mathrm{T}}\mathbf{x}) \qquad [0, 1]$

$$\boldsymbol{y = \theta(s)}$$

Linear Classification

$$\mathcal{H}_{\text{lin}} = \left\{ h(\mathbf{x}) = \text{sign}(\mathbf{w}^{\text{T}}\mathbf{x}) \right\}$$

1. $E_{\text{in}} \approx E_{\text{out}}$ because $d_{\text{VC}} = d + 1$,

$$E_{\text{out}}(h) \leq E_{\text{in}}(h) + O\left(\sqrt{\frac{d}{N}\log N}\right).$$

2. If the data is linearly separable, PLA will find a separator $\implies E_{\text{in}} = 0$.

$$\mathbf{w}(t+1) = \mathbf{w}(t) + \underset{\substack{\uparrow \\ \text{misclassified data point}}}{\mathbf{x}_* y_*}$$

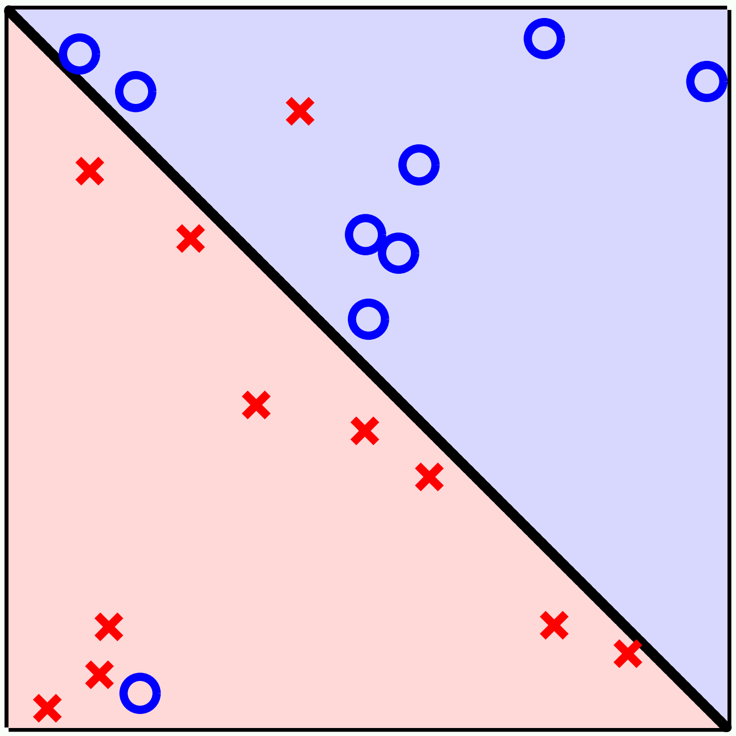
$$E_{\text{in}} = 0 \implies E_{\text{out}} \approx 0$$

(f is well approximated by a linear fit).

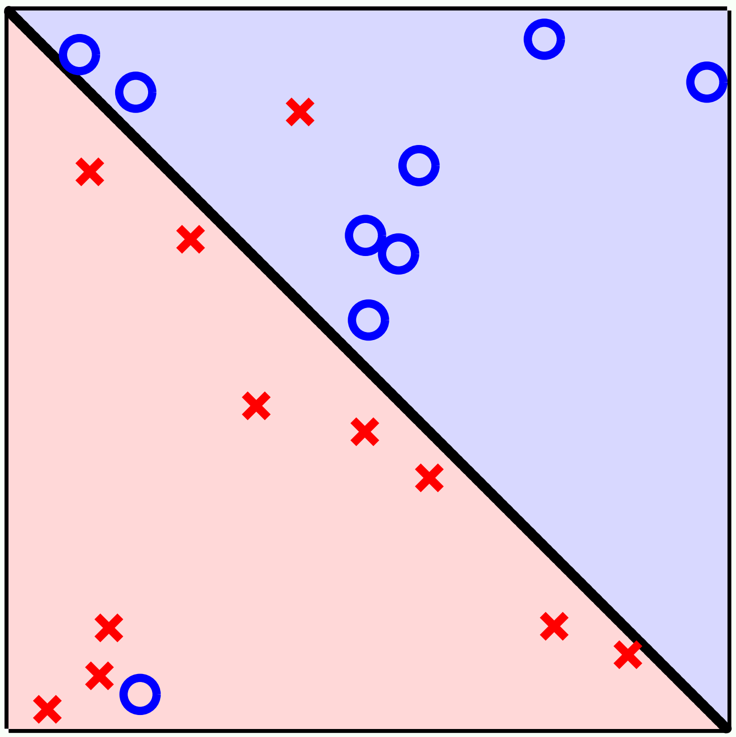
What if the data is not separable ($E_{\text{in}} = 0$ is not possible)? pocket algorithm

How to ensure $E_{\text{in}} \approx 0$ is possible? select good features

Non-Separable Data



The Pocket Algorithm



Minimizing E_{in} is a *hard* combinatorial problem.

The Pocket Algorithm

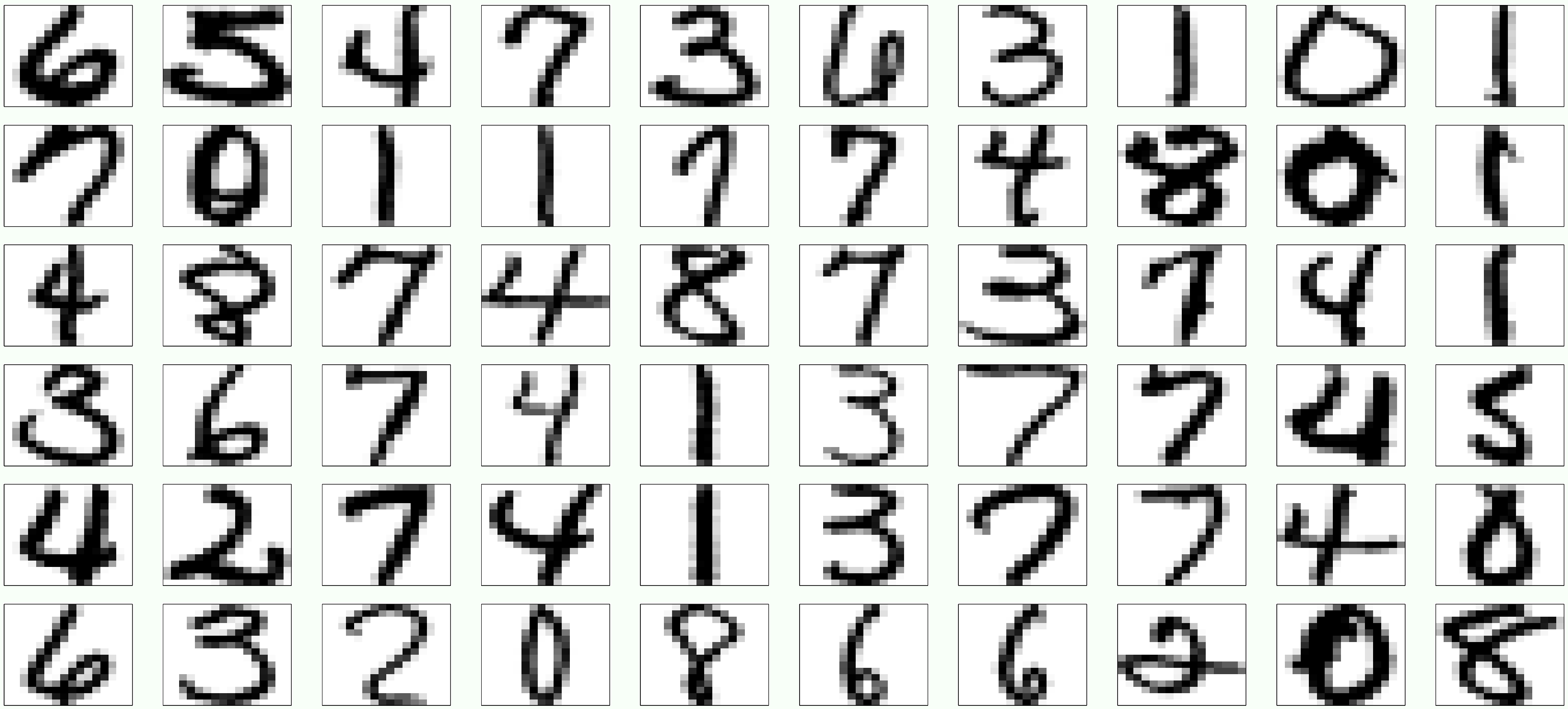
– Run PLA

– At each step keep the best E_{in} (and $\mathbf{w}$) so far.

(Its not rocket science, but it works.)

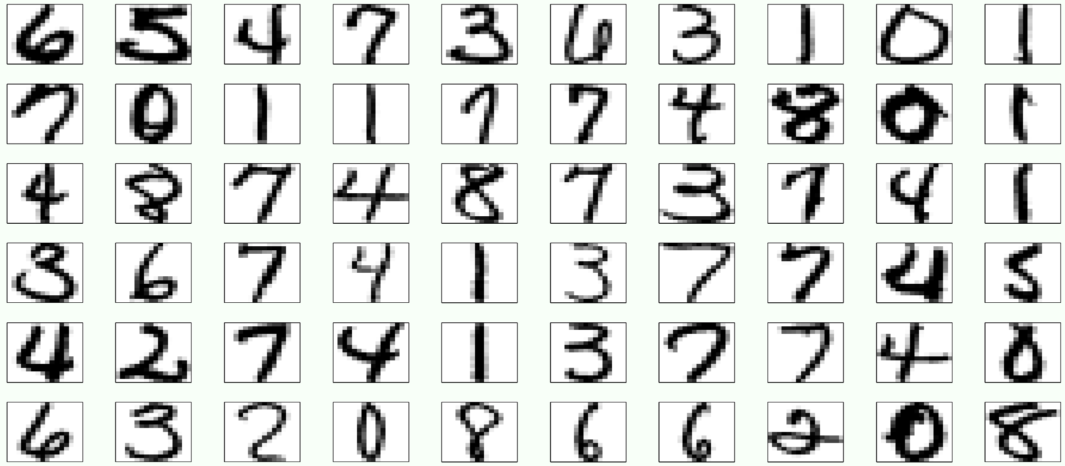
(Other approaches: linear regression, logistic regression, linear programming . . .)

Digits Data

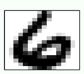


Each digit is a 16×16 image.

Digits Data



Each digit is a 16×16 image.

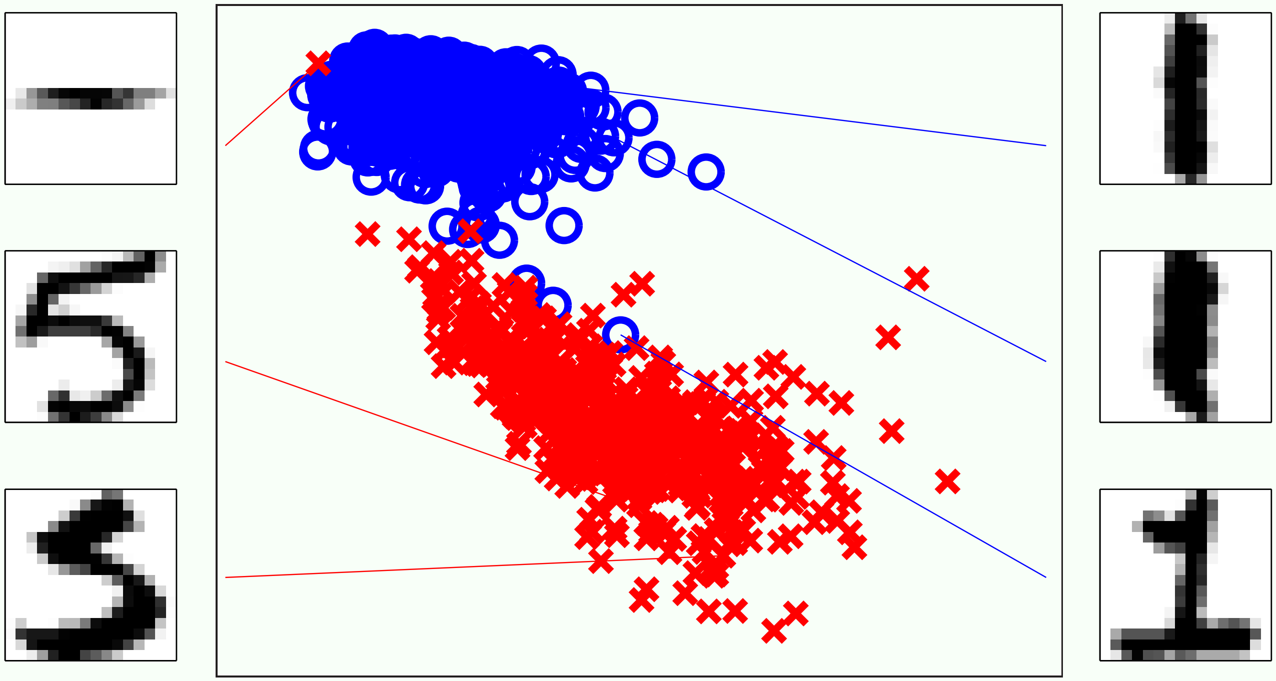


[-1 -1 -1 -1 -1 -1 -1 -0.63 0.86 -0.17 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -0.99 0.3 1 0.31 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -0.41 1 0.99 -0.57 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -0.68 0.83 1 0.56 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -0.94 0.54 1 0.78 -0.72 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 0.1 1 0.92 -0.44 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -0.26 0.95 1 -0.16 -1 -1 -1 -0.99 -0.71 -0.83 -1 -1 -1 -1 -1 -0.8 0.91 1 0.3 -0.96 -1 -1 -0.55 0.49 1 0.88 0.09 -1 -1 -1 -1 0.28 1 0.88 -0.8 -1 -0.9 0.14 0.97 1 1 1 0.99 -0.74 -1 -1 -0.95 0.84 1 0.32 -1 -1 0.35 1 0.65 -0.10 -0.18 1 0.98 -0.72 -1 -1 -0.63 1 1 0.07 -0.92 0.11 0.96 0.30 -0.88 -1 -0.07 1 0.64 -0.99 -1 -1 -0.67 1 1 0.75 0.34 1 0.70 -0.94 -1 -1 0.54 1 0.02 -1 -1 -1 -0.90 0.79 1 1 1 1 0.53 0.18 0.81 0.83 0.97 0.86 -0.63 -1 -1 -1 -1 -0.45 0.82 1 1 1 1 1 1 1 1 0.13 -1 -1 -1 -1 -1 -1 -0.48 0.81 1 1 1 1 1 1 0.21 -0.94 -1 -1 -1 -1 -1 -1 -1 -0.97 -0.42 0.30 0.82 1 0.48 -0.47 -0.99 -1 -1 -1 -1]

$$\left.\begin{array}{ll} \mathbf{x} = (1, x_1, \cdots, x_{256}) & \leftarrow \text{input} \\ \mathbf{w} = (w_0, w_1, \cdots, w_{256}) & \leftarrow \text{linear model} \end{array}\right\} d_{\text{VC}} = 257$$

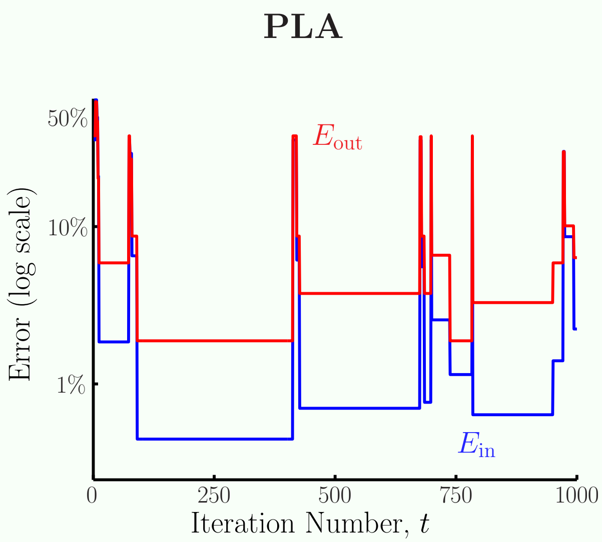
Intensity and Symmetry Features

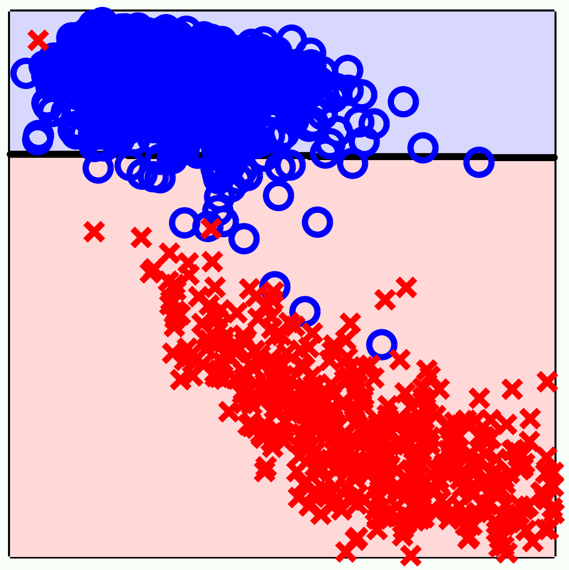
feature: an important property of the input that you think is useful for classification.
(dictionary.com: a prominent or conspicuous part or characteristic)



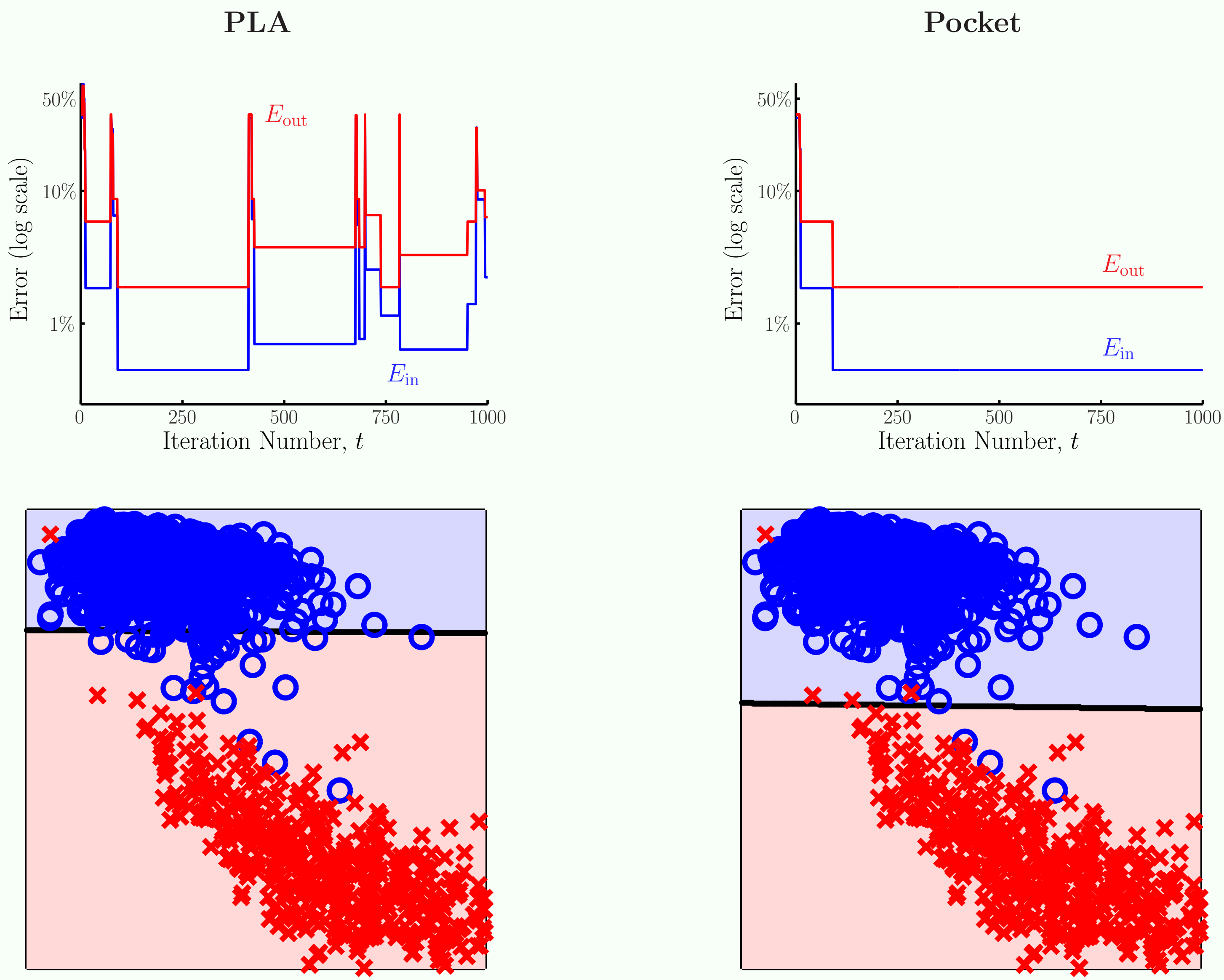
$$\left.\begin{array}{ll} \mathbf{x} = (1, x_1, x_2) & \leftarrow \text{input} \\ \mathbf{w} = (w_0, w_1, w_2) & \leftarrow \text{linear model} \end{array}\right\} d_{\text{VC}} = 3$$

PLA on Digits Data





Pocket on Digits Data



Linear Regression

age	32 years
gender	male
salary	40,000
debt	26,000
years in job	1 year
years at home	3 years
...	...

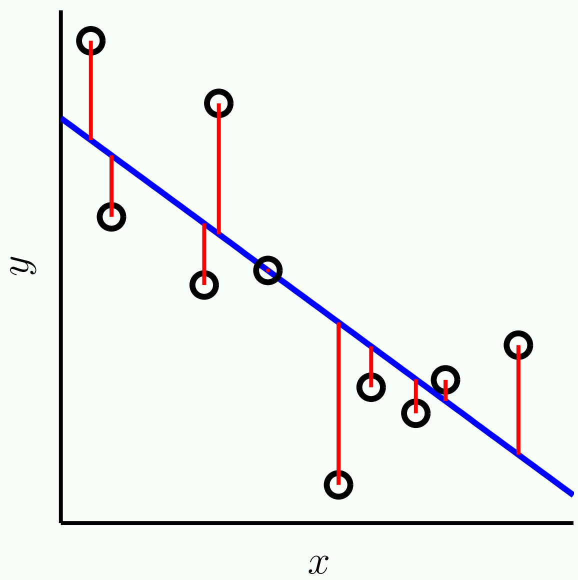
Classification: Approve/Deny

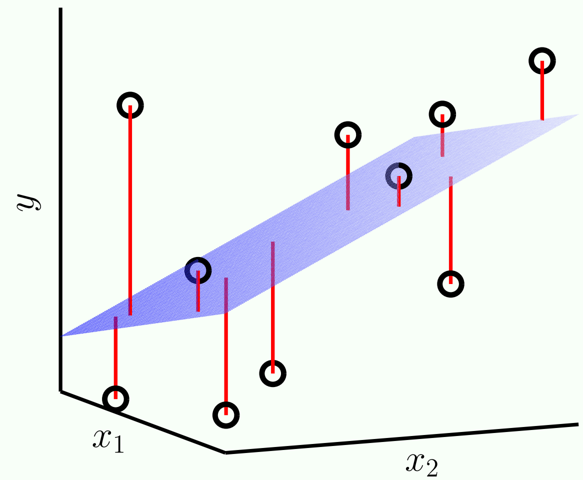
Regression: Credit Line (dollar amount)

regression $\equiv y \in \mathbb{R}$

$$h(\mathbf{x}) = \sum_{i=0}^{d} w_i x_i = \mathbf{w}^{\mathrm{T}}\mathbf{x}$$

Least Squares Linear Regression





$$y = f(\mathbf{x}) + \epsilon \qquad \longleftarrow \quad \text{noisy target } P(y|\mathbf{x})$$

in-sample error $\qquad E_{\text{in}}(h) = \frac{1}{N}\sum_{n=1}^{N}(h(\mathbf{x}_n) - y_n)^2$

out-of-sample error $\qquad E_{\text{out}}(h) = \mathbb{E}_{\mathbf{x}}[(h(\mathbf{x}) - y)^2]$

$$\left.\begin{array}{l} \\ \\ \end{array}\right\} \quad h(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x}$$

Using Matrices for Linear Regression

$$\underbrace{\mathrm{X} = \begin{bmatrix} \text{—}\mathbf{x}_1\text{—} \\ \text{—}\mathbf{x}_2\text{—} \\ \vdots \\ \text{—}\mathbf{x}_N\text{—} \end{bmatrix}}_{\text{data matrix, } N \times (d+1)} \qquad \underbrace{\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\text{target vector}} \qquad \underbrace{\hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_N \end{bmatrix} = \begin{bmatrix} \mathbf{w}^{\mathrm{T}}\mathbf{x}_1 \\ \mathbf{w}^{\mathrm{T}}\mathbf{x}_2 \\ \vdots \\ \mathbf{w}^{\mathrm{T}}\mathbf{x}_N \end{bmatrix} = \mathrm{X}\mathbf{w}}_{\text{in-sample predictions}}$$

$$\begin{aligned} E_{\text{in}}(\mathbf{w}) &= \frac{1}{N}\sum_{n=1}^{N}(\hat{y}_n - y_n)^2 \\ &= \tfrac{1}{N}\|\,\hat{\mathbf{y}} - \mathbf{y}\,\|_2^2 \\ &= \tfrac{1}{N}\|\,\mathrm{X}\mathbf{w} - \mathbf{y}\,\|_2^2 \\ &= \tfrac{1}{N}(\mathbf{w}^{\mathrm{T}}\mathrm{X}^{\mathrm{T}}\mathrm{X}\mathbf{w} - 2\mathbf{w}^{\mathrm{T}}\mathrm{X}^{\mathrm{T}}\mathbf{y} + \mathbf{y}^{\mathrm{T}}\mathbf{y}) \end{aligned}$$

Linear Regression Solution

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\left(\mathbf{w}^{\mathrm{T}}\mathrm{X}^{\mathrm{T}}\mathrm{X}\mathbf{w} - 2\mathbf{w}^{\mathrm{T}}\mathrm{X}^{\mathrm{T}}\mathbf{y} + \mathbf{y}^{\mathrm{T}}\mathbf{y}\right)$$

Vector Calculus: To minimize $E_{\text{in}}(\mathbf{w})$, set $\nabla_{\mathbf{w}} E_{\text{in}}(\mathbf{w}) = \mathbf{0}$.

$$\nabla_{\mathbf{w}}(\mathbf{w}^{\mathrm{T}}\mathrm{A}\mathbf{w}) = (\mathrm{A} + \mathrm{A}^{\mathrm{T}})\mathbf{w}, \qquad \nabla_{\mathbf{w}}(\mathbf{w}^{\mathrm{T}}\mathbf{b}) = \mathbf{b}.$$

$\mathrm{A} = \mathrm{X}^{\mathrm{T}}\mathrm{X}$ and $\mathbf{b} = \mathrm{X}^{\mathrm{T}}\mathbf{y}$:

$$\nabla_{\mathbf{w}} E_{\text{in}}(\mathbf{w}) = \frac{2}{N}(\mathrm{X}^{\mathrm{T}}\mathrm{X}\mathbf{w} - \mathrm{X}^{\mathrm{T}}\mathbf{y})$$

Setting $\nabla E_{\text{in}}(\mathbf{w}) = \mathbf{0}$:

$$\mathrm{X}^{\mathrm{T}}\mathrm{X}\mathbf{w} = \mathrm{X}^{\mathrm{T}}\mathbf{y} \qquad \longleftarrow \text{ normal equations}$$

$$\mathbf{w}_{\text{lin}} = (\mathrm{X}^{\mathrm{T}}\mathrm{X})^{-1}\mathrm{X}^{\mathrm{T}}\mathbf{y} \qquad \longleftarrow \text{ when } \mathrm{X}^{\mathrm{T}}\mathrm{X} \text{ is invertible}$$

Linear Regression Algorithm

Linear Regression Algorithm:

1. Construct the matrix X and the vector $\mathbf{y}$ from the data set $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$, where each $\mathbf{x}$ includes the $x_0 = 1$ coordinate,

$$\underbrace{\mathrm{X} = \begin{bmatrix} \text{—}\mathbf{x}_1\text{—} \\ \text{—}\mathbf{x}_2\text{—} \\ \vdots \\ \text{—}\mathbf{x}_N\text{—} \end{bmatrix}}_{\text{data matrix}}, \qquad \underbrace{\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\text{target vector}}.$$

2. Compute the pseudo inverse $\mathrm{X}^\dagger$ of the matrix X. If $\mathrm{X}^{\mathrm{T}}\mathrm{X}$ is invertible,

$$\mathrm{X}^\dagger = (\mathrm{X}^{\mathrm{T}}\mathrm{X})^{-1}\mathrm{X}^{\mathrm{T}}$$

3. Return $\mathbf{w}_{\text{lin}} = \mathrm{X}^\dagger\mathbf{y}$.

Generalization

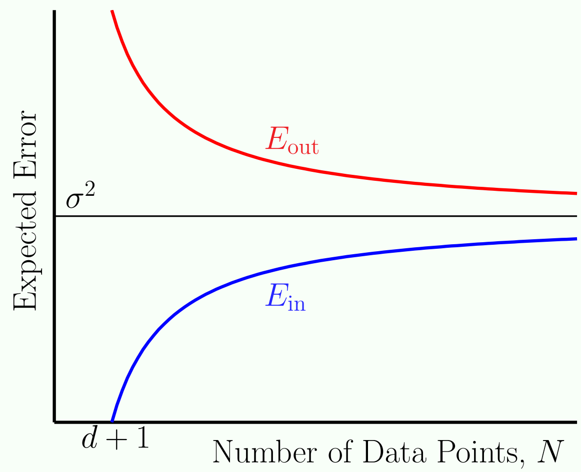
The linear regression algorithm gets the smallest possible E_{in} in *one step*.

Generalization is also good.

One can obtain a regression version of d_{VC}.

There are other bounds, for example:

$$\mathbb{E}[E_{\text{out}}(h)] = \mathbb{E}[E_{\text{in}}(h)] + O\left(\frac{d}{N}\right)$$



Linear Regression for Classification

Linear regression can learn *any* real valued target function.

For example $y_n = \pm 1$. (± 1 are real values!)

Use linear regression to get $\mathbf{w}$ with $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n \approx y_n = \pm 1$

Then $\text{sign}(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n)$ will likely agree with $y_n = \pm 1$.

These can be good initial weights for classification.

Example.

Classifying 1 from not 1

(multiclass $\rightarrow$ 2 class)